DL-Alanine, N-methyl-N-octyloxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C27H53NO4/c1-5-7-9-11-13-14-15-16-17-18-20-21-23-31-26(29)25(3)28(4)27(

InchiKey: OALQOOJJSWGEIL-UHFFFAOYSA-N

Formula: C27H53NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCC

Mol. weight [g/mol]: 455.71

Physical Properties

Property code	Value	Unit	Source
gf	-183.04	kJ/mol	Joback Method
hf	-1027.96	kJ/mol	Joback Method
hfus	70.76	kJ/mol	Joback Method
hvap	95.66	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	8.048		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	725.75	kPa	Joback Method
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
tb	981.74	K	Joback Method
tc	1215.30	K	Joback Method
tf	555.84	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.24	J/mol×K	981.74	Joback Method
cpg	1477.43	J/mol×K	1020.67	Joback Method
cpg	1497.70	J/mol×K	1059.59	Joback Method
cpg	1516.15	J/mol×K	1098.52	Joback Method
cpg	1532.85	J/mol×K	1137.44	Joback Method
cpg	1547.86	J/mol×K	1176.37	Joback Method
cpg	1561.28	J/mol×K	1215.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume